



# wwPDB Geometry-Only Validation Summary Report ⓘ

May 23, 2024 – 09:23 AM EDT

PDB ID : 2INQ  
Title : Neutron Crystal Structure of Escherichia coli Dihydrofolate Reductase Bound to the Anti-cancer drug, Methotrexate  
Authors : Bennett, B.C.; Langan, P.A.; Coates, L.; Schoenborn, B.; Dealwis, C.G.  
Deposited on : 2006-10-08  
Resolution : 2.20 Å (reported)

This is a wwPDB Geometry-Only Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

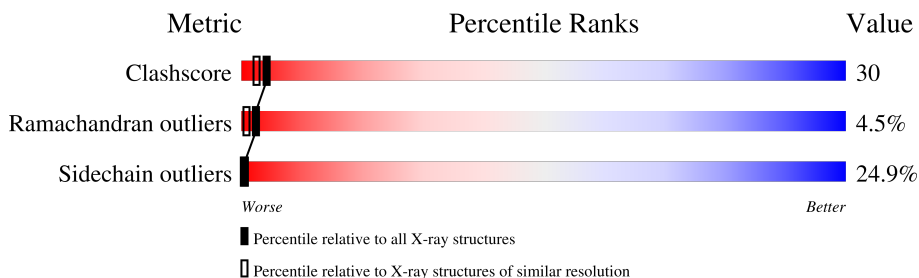
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*NEUTRON DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	159	 40% 44% 16%
1	B	159	 35% 51% 13% .

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5476 atoms, of which 2147 are hydrogens and 595 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

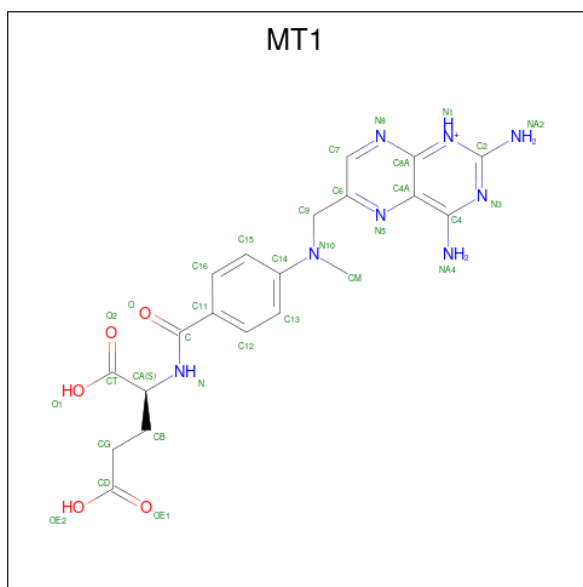
- Molecule 1 is a protein called Dihydrofolate reductase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	159	2452	800	146	1052	213	234	7	0	0	0
1	B	159	2478	803	157	1059	216	236	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	engineered mutation	UNP P0ABQ4
B	37	ASP	ASN	engineered mutation	UNP P0ABQ4

- Molecule 2 is N-(4-[(2,4-DIAMINOPTERIDIN-1-IUM-6-YL)METHYL](METHYL)AMINO}BENZOYL)-L-GLUTAMIC ACID (three-letter code: MT1) (formula: C<sub>20</sub>H<sub>23</sub>N<sub>8</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	D	H	N	O		
2	A	1	53	20	2	18	8	5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	D	H	N			O
2	B	1	53	20	2	18	8	5	0	0

- Molecule 3 is water.

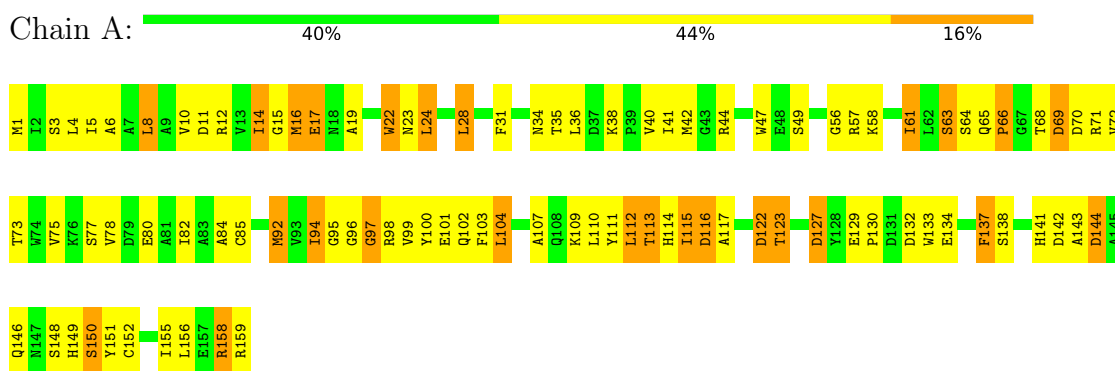
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	D	O		
3	A	65	183	118	65	0	0
3	B	87	257	170	87	0	0

### 3 Residue-property plots [i](#)

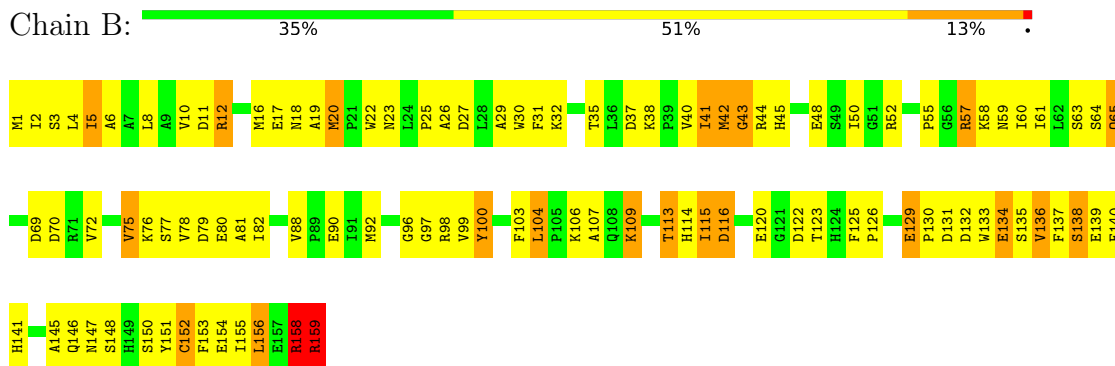
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: Dihydrofolate reductase



- Molecule 1: Dihydrofolate reductase



## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MT1, DOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.52	0/1286	0.96	3/1747 (0.2%)
1	B	0.51	0/1296	1.04	10/1762 (0.6%)
All	All	0.52	0/2582	1.00	13/3509 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	159	ARG	NE-CZ-NH2	-10.73	114.94	120.30
1	B	12	ARG	NE-CZ-NH1	-10.36	115.12	120.30
1	B	158	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	B	158	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	158	ARG	NH1-CZ-NH2	8.08	128.29	119.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	63	SER	Peptide

## 4.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1400	1052	1201	87	0
1	B	1419	1059	1217	70	0
2	A	35	18	21	1	0
2	B	35	18	21	1	0
3	A	183	0	0	6	0
3	B	257	0	0	6	0
All	All	3329	2147	2460	149	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

The worst 5 of 149 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASP:OD2	1:A:150:SER:HB3	1.33	1.21
1:A:12:ARG:HH22	1:A:127:ASP:CG	1.68	0.93
1:A:71:ARG:CB	1:A:71:ARG:C	2.50	0.80
1:A:116:ASP:OD2	1:A:150:SER:CB	2.25	0.80
1:A:71:ARG:CB	1:A:71:ARG:N	2.45	0.79

There are no symmetry-related clashes.

## 4.3 Torsion angles [i](#)

### 4.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	156/159 (98%)	121 (78%)	26 (17%)	9 (6%)	<b>1</b> <b>0</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	157/159 (99%)	124 (79%)	28 (18%)	5 (3%)	4	2
All	All	313/318 (98%)	245 (78%)	54 (17%)	14 (4%)	2	1

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	THR
1	A	97	GLY
1	A	17	GLU
1	B	129	GLU
1	A	64	SER

#### 4.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/136 (96%)	103 (79%)	28 (21%)	1	1
1	B	134/136 (98%)	96 (72%)	38 (28%)	0	0
All	All	265/272 (97%)	199 (75%)	66 (25%)	0	0

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	134	GLU
1	B	136	VAL
1	B	159	ARG
1	A	144	ASP
1	A	142	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	65	GLN

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Mol	Chain	Res	Type
1	A	149	HIS

#### 4.3.3 RNA [i](#)

There are no RNA molecules in this entry.

#### 4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

#### 4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

#### 4.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MT1	B	1147	-	35,35,35	2.09	10 (28%)	46,49,49	3.04	20 (43%)
2	MT1	A	1146	-	35,35,35	1.62	8 (22%)	46,49,49	2.92	14 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MT1	B	1147	-	-	3/25/25/25	0/3/3/3
2	MT1	A	1146	-	-	3/25/25/25	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1147	MT1	C4A-C8A	-6.53	1.29	1.40
2	A	1146	MT1	C4A-C8A	-4.32	1.32	1.40
2	B	1147	MT1	C8A-N1	3.76	1.44	1.36
2	B	1147	MT1	C2-NA2	-3.73	1.26	1.33
2	B	1147	MT1	C16-C15	-3.69	1.32	1.38

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1146	MT1	C4A-C4-N3	-13.63	112.06	121.01
2	B	1147	MT1	C4A-C4-N3	-12.13	113.04	121.01
2	B	1147	MT1	N1-C2-N3	-8.94	115.29	127.22
2	A	1146	MT1	N1-C2-N3	-7.54	117.16	127.22
2	B	1147	MT1	C7-C6-N5	-4.31	118.03	120.85

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1146	MT1	C6-C9-N10-CM
2	B	1147	MT1	C6-C9-N10-CM
2	A	1146	MT1	OE2-CD-CG-CB
2	A	1146	MT1	OE1-CD-CG-CB
2	B	1147	MT1	OE2-CD-CG-CB

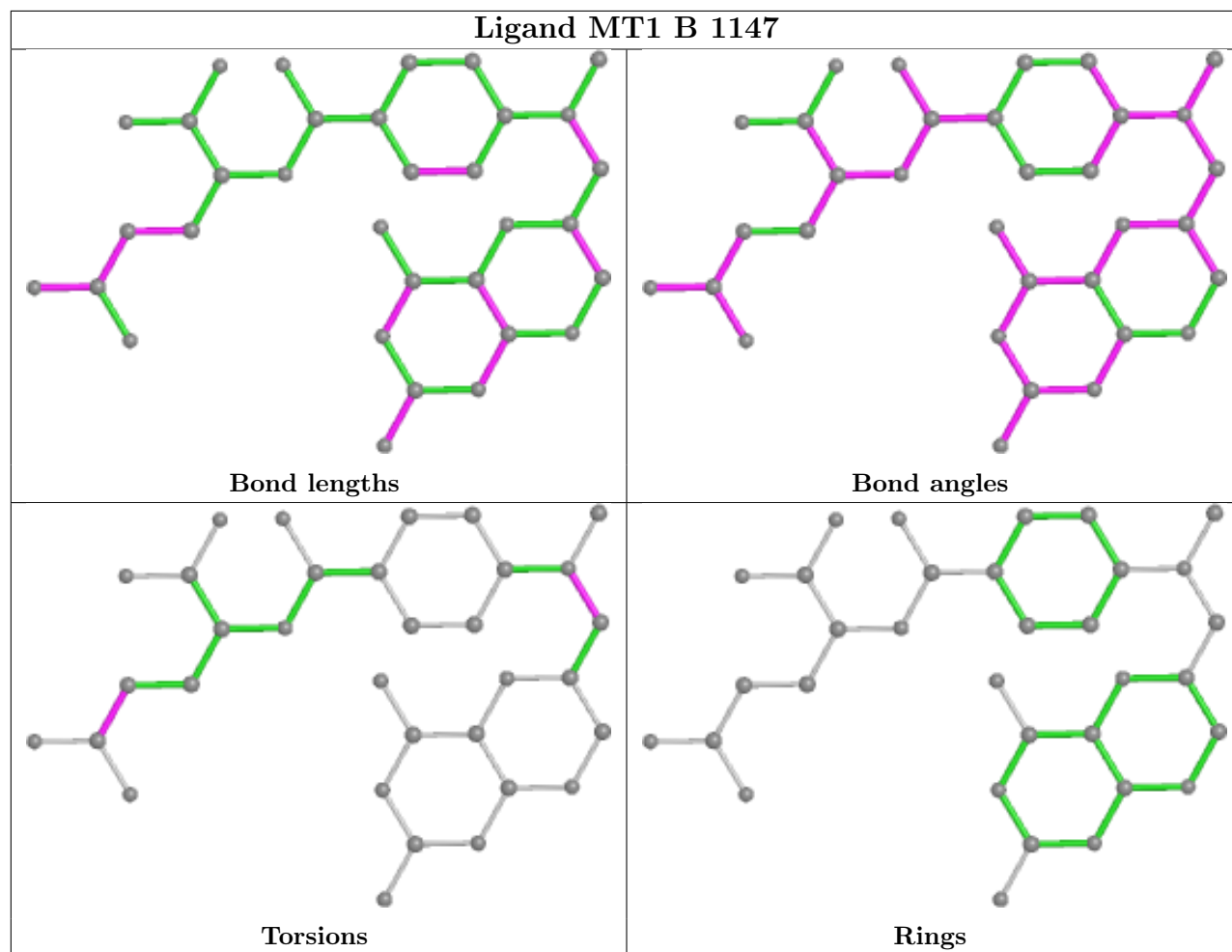
There are no ring outliers.

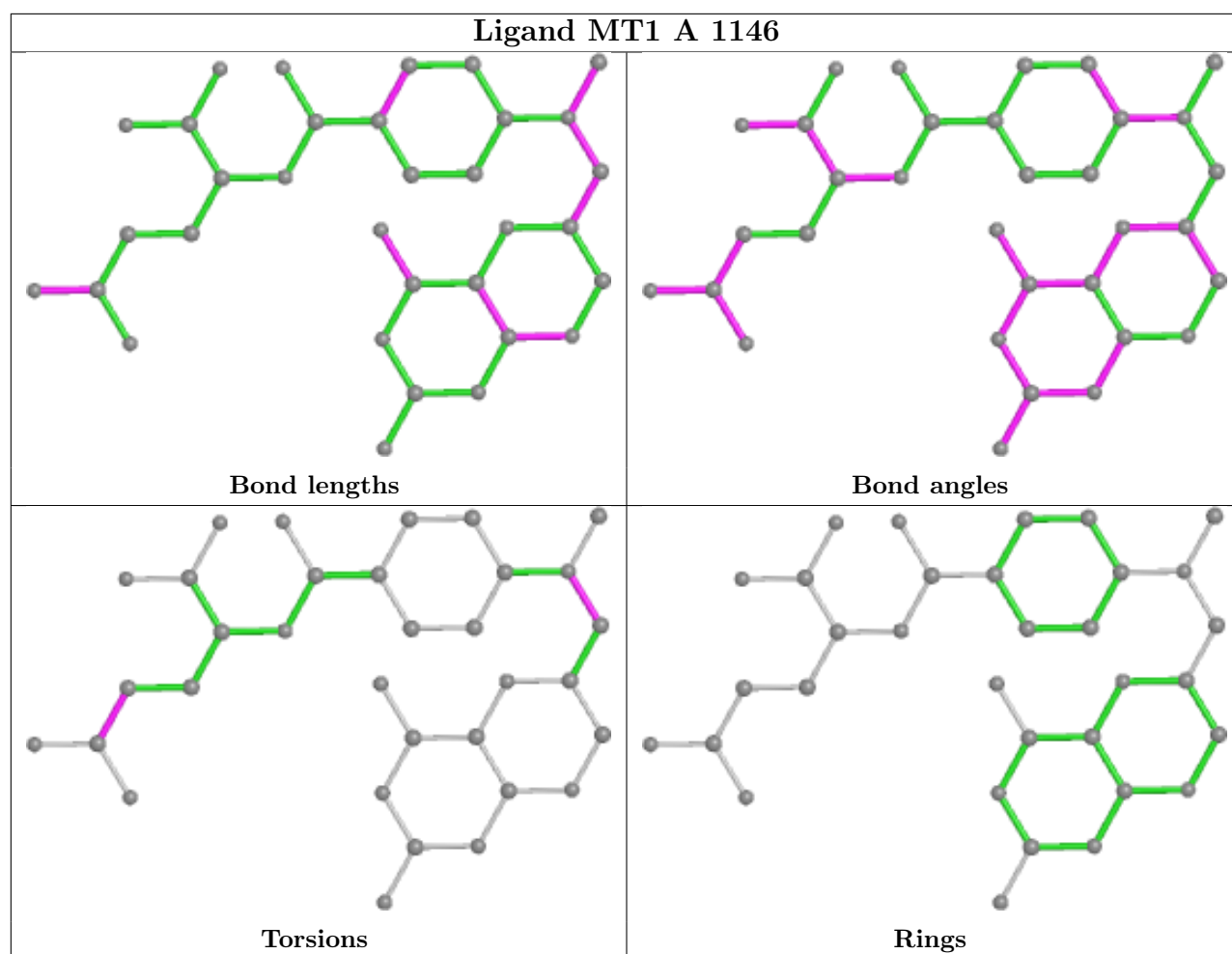
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1147	MT1	1	0
2	A	1146	MT1	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





#### 4.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.